In[1]:=

Appendix A

In[2]:= Kyle Cranmer, Sven Kreiss, David López - Val, and Tilman Plehn

- **Define log likelihood for Appendix A (Eq. A1 & A2)**

In[2]:=
```
nu[mu1_, mu2_, s1_, s2_, alpha_, b_] :=
 mu1 * s1 * (1 + eta11 alpha) + mu2 * s2 * (1 + eta12 alpha) + b
```

In[3]:=
```
nu2[mu1_, mu2_, s1_, s2_, alpha_, b_] :=
 mu1 * s1 * (1 + eta21 alpha) + mu2 * s2 * (1 + eta22 alpha) + b
```

In[4]:=
```
l[x1_, m1_, s1_, x2_, m2_, s2_, alpha_] :=
 (x1 - m1 ) ^2 / (2 s1^2) + (x2 - m2) ^2 / (2 s2^2) + (alpha) ^2 / (2 sa^2)
```

In[5]:=
```
L = l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
    x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha];
```

- **Solve Conditioanl MLE mufix (Equation 2.20)**

In[6]:=
```
CMLE = Simplify[Solve[D[
      l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
       x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha], {{mu1, mu2}, 1}] == 0, {mu1, mu2}]]
```

Out[6]=
```
{{mu1 → (b2 (s12 + alpha eta12 s12) - b1 (s22 + alpha eta22 s22) +
        s22 x1 + alpha eta22 s22 x1 - s12 x2 - alpha eta12 s12 x2) /
      (- (1 + alpha eta12) (1 + alpha eta21) s12 s21 + (1 + alpha eta11) (1 + alpha eta22) s11 s22),
   mu2 → (-b2 (s11 + alpha eta11 s11) + b1 (s21 + alpha eta21 s21) -
        s21 x1 - alpha eta21 s21 x1 + s11 x2 + alpha eta11 s11 x2) /
      (- (1 + alpha eta12) (1 + alpha eta21) s12 s21 + (1 + alpha eta11) (1 + alpha eta22) s11 s22)}}
```

- **Solve MLE (Equation A.3)**

For some reason, Mathematica has a hard time solving for the MLE, help it out by hand

MLE = Simplify[Solve[D[
  l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
   x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha], {{mu1, mu2}, 1}] == 0, {mu1, mu2, alpha}]]

In[7]:=
```
MLE = {{0, 0, 0}, {CMLE[[1, 1]] /. alpha → 0, CMLE[[1, 2]] /. alpha → 0, alpha → 0}}
```

Out[7]=

$$\left\{\{0,0,0\},\ \left\{mu1 \to \frac{b2\ s12 - b1\ s22 + s22\ x1 - s12\ x2}{-s12\ s21 + s11\ s22},\ mu2 \to \frac{-b2\ s11 + b1\ s21 - s21\ x1 + s11\ x2}{-s12\ s21 + s11\ s22},\ alpha \to 0\right\}\right\}$$

- **Equation 2.21 Derivative of CMLE mufix wrt. alpha is - eta_p muhat_p (independent of sa)**

In[8]:=
```
Eta1PartialSolution = Simplify[D[CMLE[[1, 1, 2]], alpha] / MLE[[2, 1, 2]] /. alpha → 0]
```

Out[8]=

$$\big((-s12\ s21 + s11\ s22)\big((eta12\ s12\ s21 + eta21\ s12\ s21 - (eta11 + eta22)\ s11\ s22)(b2\ s12 - b1\ s22 + s22\ x1 - s12\ x2) + (-s12\ s21 + s11\ s22)(b2\ eta12\ s12 - b1\ eta22\ s22 + eta22\ s22\ x1 - eta12\ s12\ x2)\big)\big) \Big/ \Big((s12\ s21 - s11\ s22)^2\ (b2\ s12 - b1\ s22 + s22\ x1 - s12\ x2)\Big)$$

In[9]:=
```
Eta2PartialSolution = Simplify[D[CMLE[[1, 2, 2]], alpha] / MLE[[2, 2, 2]] /. alpha → 0]
```

Out[9]=

$$\big((-s12\ s21 + s11\ s22)\big((eta12\ s12\ s21 + eta21\ s12\ s21 - (eta11 + eta22)\ s11\ s22)(-b2\ s11 + b1\ s21 - s21\ x1 + s11\ x2) + (-s12\ s21 + s11\ s22)(-b2\ eta11\ s11 + b1\ eta21\ s21 - eta21\ s21\ x1 + eta11\ s11\ x2)\big)\big) \Big/ \Big((s12\ s21 - s11\ s22)^2\ (-b2\ s11 + b1\ s21 - s21\ x1 + s11\ x2)\Big)$$

Show that Solution in category universal situation is as expected

In[10]:=
```
Simplify[Eta1PartialSolution /. {alpha → 0,
    s11 → 90, s12 → 10, x1 → 100,
    x21 → 10, s22 → 90, x2 → 100,
    eta11 → eta1, eta21 → eta1, eta12 → eta2, eta22 → eta2}]
```

Out[10]= −eta1

- **Equation 2.15 Calculate the fisher info matrices for full likelihood (w/ full dependence or evaluated at MLE)**

In[11]:=
```
Ifull = Simplify[D[l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
      x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha], {{mu1, mu2, alpha}, 2}]];
```

In[12]:=
```
IfullAtMLE = Simplify[D[l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
        x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha], {{mu1, mu2, alpha}, 2}] /. MLE[[2]]
    alpha → 0] ;
```

- **Show that the conditional MVG equations are equivalent to dmu_p^fix /dalpha. Note the independence on sa (uncertainty on alpha)**

- **Equation 2.23: Calculate the full covariance matrix Sigma**

In[13]:=
```
Sigma = Simplify[Inverse[IfullAtMLE]] ;
```

In[14]:=
```
Sigma33 = Sigma[[3, 3]]
```

Out[14]= sa^2

Equation 2.22

In[15]:=
```
Eta2CovSolution = Simplify[Sigma[[2, 3]] / Sigma[[3, 3]] / MLE[[2, 2, 2]]]
```

Out[15]=
$$\Big(b2\,s11\,(-eta11\,s12\,s21+eta12\,s12\,s21+eta21\,s12\,s21-eta22\,s11\,s22)+b1\,s21\,(-eta12\,s12\,s21+(eta11-eta21+eta22)\,s11\,s22)+eta12\,s12\,s21^2\,x1-eta11\,s11\,s21\,s22\,x1+eta21\,s11\,s21\,s22\,x1-eta22\,s11\,s21\,s22\,x1+eta11\,s11\,s12\,s21\,x2-eta12\,s11\,s12\,s21\,x2-eta21\,s11\,s12\,s21\,x2+eta22\,s11^2\,s22\,x2\Big)\Big/\big((s12\,s21-s11\,s22)\,(-b2\,s11+b1\,s21-s21\,x1+s11\,x2)\big)$$

In[16]:=
```
Simplify[Eta2PartialSolution - Eta2CovSolution]
```

Out[16]= 0

- **Show that the information matrix approach is equivalent**

a) Get IfullAtMLE
b) get Ieff
c) solve for effective etas
Try to show :
1) if Imain=Ifull for other elements
2) if solution to effective etas is the same as the muhat derivative symbolically

Equation 2.15

In[17]:=
```
Ieff = Simplify[D[l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
      x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha], {{mu1, mu2}, 2}] ];
```

- **Eq. A6 : Calculate the effective fisher info matrix (w/ full dependence or evaluated at MLE)**

In[18]:=
```
IeffAtMLE = Simplify[D[l[x1, nu[mu1, mu2, s11, s12, alpha, b1], s1,
       x2, nu2[mu1, mu2, s21, s22, alpha, b2], s2, alpha], {{mu1, mu2}, 2}] /. MLE[[2]]];
```

In[19]:=
```
Simplify[Inverse[IeffAtMLE]]
```

Out[19]=
$$\left\{\left\{\frac{s12^2\, s2^2 + s1^2\, s22^2}{(s12\, s21 - s11\, s22)^2}, -\frac{s11\, s12\, s2^2 + s1^2\, s21\, s22}{(s12\, s21 - s11\, s22)^2}\right\}, \left\{-\frac{s11\, s12\, s2^2 + s1^2\, s21\, s22}{(s12\, s21 - s11\, s22)^2}, \frac{s11^2\, s2^2 + s1^2\, s21^2}{(s12\, s21 - s11\, s22)^2}\right\}\right\}$$

- **Eq 2.9: Define the mu_eff substitution, calculate Jacobian, reparametrize Ieff -> Imain**

In[20]:=
```
mueff[mu1_, mu2_, alpha_] := List[mu1 (1 + eta1 alpha), mu2 ( 1 + eta2 alpha)]
```

Eq A8

In[21]:=
```
J = D[mueff[mu1, mu2, alpha], {{mu1, mu2, alpha}, 1}]
```

Out[21]=
$$\{\{1 + alpha\, eta1, 0, eta1\, mu1\}, \{0, 1 + alpha\, eta2, eta2\, mu2\}\}$$

Eq A9

In[22]:=
```
Imain = Simplify[Transpose[J].IeffAtMLE.J] ;
```

In[23]:=
```
Imain /. alpha → 0
```

Out[23]=
$$\left\{\left\{\frac{s11^2}{s1^2} + \frac{s21^2}{s2^2}, \frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}, eta1\, mu1 \left(\frac{s11^2}{s1^2} + \frac{s21^2}{s2^2}\right) + eta2\, mu2 \left(\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}\right)\right\},\right.$$
$$\left\{\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}, \frac{s12^2}{s1^2} + \frac{s22^2}{s2^2}, eta1\, mu1 \left(\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}\right) + eta2\, mu2 \left(\frac{s12^2}{s1^2} + \frac{s22^2}{s2^2}\right)\right\},$$
$$\left\{eta1\, mu1 \left(\frac{s11^2}{s1^2} + \frac{s21^2}{s2^2}\right) + eta2\, mu2 \left(\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}\right),\right.$$
$$eta1\, mu1 \left(\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}\right) + eta2\, mu2 \left(\frac{s12^2}{s1^2} + \frac{s22^2}{s2^2}\right), \frac{1}{s1^2\, s2^2} \Big(eta1^2\, mu1^2 \left(s11^2\, s2^2 + s1^2\, s21^2\right) +$$
$$\left.\left. 2\, eta1\, eta2\, mu1\, mu2 \left(s11\, s12\, s2^2 + s1^2\, s21\, s22\right) + eta2^2\, mu2^2 \left(s12^2\, s2^2 + s1^2\, s22^2\right)\Big)\right\}\right\}$$

In[24]:=
```
Iconstr = {{0, 0, 0}, {0, 0, 0}, {0, 0, 1 / sa^2}}
```

Out[24]=
$$\left\{\{0, 0, 0\}, \{0, 0, 0\}, \left\{0, 0, \frac{1}{sa^2}\right\}\right\}$$

- **Show solution to eta's is indeed solution of linear equations RHS=from full model, LHS=reparametrizing L_eff->L_main**

Eq A.4

In[25]:=
```
RHS13 = IfullAtMLE[[1, 3]]  /. alpha → 0
```

Out[25]=
$$\frac{1}{s1^2\, s2^2\, (s12\, s21 - s11\, s22)}$$
$$\Big(b1 \left(-eta12\, s11\, s12\, s2^2\, s21 + \left(eta11\, s11^2\, s2^2 + (eta21 - eta22)\, s1^2\, s21^2\right) s22\right) +$$
$$b2 \left(-eta11\, s11^2\, s12\, s2^2 + eta12\, s11^2\, s12\, s2^2 + s1^2\, s21\, (-eta21\, s12\, s21 + eta22\, s11\, s22)\right) +$$
$$eta12\, s11\, s12\, s2^2\, s21\, x1 - eta11\, s11^2\, s2^2\, s22\, x1 - eta21\, s1^2\, s21^2\, s22\, x1 + eta22\, s1^2\, s21^2\, s22\, x1 +$$
$$eta11\, s11^2\, s12\, s2^2\, x2 - eta12\, s11^2\, s12\, s2^2\, x2 + eta21\, s1^2\, s12\, s21^2\, x2 - eta22\, s1^2\, s11\, s21\, s22\, x2\Big)$$

In[26]:=
```
RHS23 = IfullAtMLE[[2, 3]] /. alpha → 0
```

Out[26]=
$$\frac{1}{s1^2\, s2^2\, (s12\, s21 - s11\, s22)} \Big(b2 \left(-eta11\, s11\, s12^2\, s2^2 + eta12\, s11\, s12^2\, s2^2 + s1^2\, s22\, (-eta21\, s12\, s21 + eta22\, s11\, s22)\right) + b1 \left(-eta12\, s12^2\, s2^2\, s21 + s22 \left(eta11\, s11\, s12\, s2^2 + (eta21 - eta22)\, s1^2\, s21\, s22\right)\right) + eta12\, s12^2\, s2^2\, s21\, x1 - eta11\, s11\, s12\, s2^2\, s22\, x1 - eta21\, s1^2\, s21\, s22^2\, x1 + eta22\, s1^2\, s21\, s22^2\, x1 + eta11\, s11\, s12^2\, s2^2\, x2 - eta12\, s11\, s12^2\, s2^2\, x2 + eta21\, s1^2\, s12\, s21\, s22\, x2 - eta22\, s1^2\, s11\, s22^2\, x2\Big)$$

introduce "unk1" the unknowns we want to solve for

In[27]:=
```
LHS13 = Imain[[1, 3]] /. {alpha → 0, eta1 → unk1, eta2 → unk2}
```

Out[27]=
$$mu1 \left(\frac{s11^2}{s1^2} + \frac{s21^2}{s2^2}\right) unk1 + mu2 \left(\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}\right) unk2$$

In[28]:=
```
LHS23 = Imain[[2, 3]] /. {alpha → 0, eta1 → unk1, eta2 → unk2}
```

Out[28]=
$$mu1 \left(\frac{s11\, s12}{s1^2} + \frac{s21\, s22}{s2^2}\right) unk1 + mu2 \left(\frac{s12^2}{s1^2} + \frac{s22^2}{s2^2}\right) unk2$$

Eq. A .9 & A .11

In[29]:=
```
EtaInfoSolutions = Solve[{LHS13 == RHS13, LHS23 == RHS23}, {unk1, unk2}] /. MLE[[2]] /.
  {alpha → 0, unk1 → eta1, unk2 → eta2}
```

Out[29]=
$$\Big\{\Big\{eta1 \to -\Big((-s12\, s21 + s11\, s22) \big(b2\, eta21\, s12^2\, s21 - b2\, eta11\, s11\, s12\, s22 + b2\, eta12\, s11\, s12\, s22 - b2\, eta22\, s11\, s12\, s22 - b1\, eta12\, s12\, s21\, s22 - b1\, eta21\, s12\, s21\, s22 + b1\, eta22\, s12\, s21\, s22 + b1\, eta11\, s11\, s22^2 + eta12\, s12\, s21\, s22\, x1 + eta21\, s12\, s21\, s22\, x1 - eta22\, s12\, s21\, s22\, x1 - eta11\, s11\, s22^2\, x1 - eta21\, s12^2\, s21\, x2 + eta11\, s11\, s12\, s22\, x2 - eta12\, s11\, s12\, s22\, x2 + eta22\, s11\, s12\, s22\, x2\big)\Big) \Big/ \Big((s12\, s21 - s11\, s22)^2\, (b2\, s12 - b1\, s22 + s22\, x1 - s12\, x2)\Big),$$
$$eta2 \to -\Big((-s12\, s21 + s11\, s22) \big(b2\, eta11\, s11\, s12\, s21 - b2\, eta12\, s11\, s12\, s21 - b2\, eta21\, s11\, s12\, s21 + b1\, eta12\, s12\, s21^2 + b2\, eta22\, s11^2\, s22 - b1\, eta11\, s11\, s21\, s22 + b1\, eta21\, s11\, s21\, s22 - b1\, eta22\, s11\, s21\, s22 - eta12\, s12\, s21^2\, x1 + eta11\, s11\, s21\, s22\, x1 - eta21\, s11\, s21\, s22\, x1 + eta22\, s11\, s21\, s22\, x1 - eta11\, s11\, s12\, s21\, x2 + eta12\, s11\, s12\, s21\, x2 + eta21\, s11\, s12\, s21\, x2 - eta22\, s11^2\, s22\, x2\big)\Big) \Big/ \Big((s12\, s21 - s11\, s22)^2\, (-b2\, s11 + b1\, s21 - s21\, x1 + s11\, x2)\Big)\Big\}\Big\}$$

This shows that eta from derivative is equal to eta from fisher info approach

In[30]:=
```
Simplify[Simplify[-D[CMLE[[1, 1, 2]], alpha] / MLE[[2, 1, 2]] /. alpha → 0] - eta1 /.
  EtaInfoSolutions[[1]]]
```

Out[30]= 0

In[31]:=
```
Simplify[Simplify[-D[CMLE[[1, 2, 2]], alpha] / MLE[[2, 2, 2]] /. alpha → 0] - eta2 /.
  EtaInfoSolutions[[1]]]
```

Out[31]= 0

Same idea, but in terms of arbitrary elemnts of IeffAtMLE

In[32]:=
```
IeffArb = {{Imain11, Imain12}, {Imain12, Imain22}}
```

Out[32]= {{Imain11, Imain12}, {Imain12, Imain22}}

In[33]:=
```
ImainArb = Simplify[Transpose[J].IeffArb.J]
```

Out[33]=
```
{{(1 + alpha eta1)^2 Imain11, (1 + alpha eta1) (1 + alpha eta2) Imain12,
  (1 + alpha eta1) (eta1 Imain11 mu1 + eta2 Imain12 mu2)},
 {(1 + alpha eta1) (1 + alpha eta2) Imain12, (1 + alpha eta2)^2 Imain22,
  (1 + alpha eta2) (eta1 Imain12 mu1 + eta2 Imain22 mu2)},
 {(1 + alpha eta1) (eta1 Imain11 mu1 + eta2 Imain12 mu2),
  (1 + alpha eta2) (eta1 Imain12 mu1 + eta2 Imain22 mu2),
  eta1^2 Imain11 mu1^2 + 2 eta1 eta2 Imain12 mu1 mu2 + eta2^2 Imain22 mu2^2}}
```

In[34]:=
```
LHS13Raw = ImainArb[[1, 3]] /. {alpha → 0, eta1 → unk1, eta2 → unk2}
```

Out[34]=
```
Imain11 mu1 unk1 + Imain12 mu2 unk2
```

In[35]:=
```
LHS23Raw = ImainArb[[2, 3]] /. {alpha → 0, eta1 → unk1, eta2 → unk2}
```

Out[35]=
```
Imain12 mu1 unk1 + Imain22 mu2 unk2
```

In[36]:=
```
Solve[{LHS13Raw == I13, LHS23Raw == I23}, {unk1, unk2}]
```

Out[36]=

$$\left\{\left\{unk1 \to -\frac{-I23\ Imain12 + I13\ Imain22}{\left(Imain12^2 - Imain11\ Imain22\right)\ mu1},\ unk2 \to -\frac{I23\ Imain11 - I13\ Imain12}{\left(Imain12^2 - Imain11\ Imain22\right)\ mu2}\right\}\right\}$$

- **Fig 7: Compare Lfull to recoupled model (from substitution of mueff into the Leff) for Scenarios A,B,C**

In[37]:=
```
arg = Simplify[{{MLE[[2, 1, 2]] - mu1 (1 + eta1 alpha), MLE[[2, 2, 2]] - mu2 (1 + eta2 alpha)}} /.
    EtaInfoSolutions[[1]]] ;
```

In[38]:=
```
leff = arg.IeffAtMLE.Transpose[arg] / 2 + alpha^2 / (2 sa^2);
```

Try to profile alpha and repeat

In[39]:=
```
AlphaFullProfile = Solve[D[L, {alpha, 1}] == 0, {alpha}][[1]] ;
```

In[40]:=
```
AlphaEffProfile = Solve[D[leff, {alpha, 1}] == 0, {alpha}][[1]] ;
```

In[41]:=
```
leffProfiled = leff /. AlphaEffProfile ;
```

In[42]:=
```
LProfiled = L /. AlphaFullProfile ;
```

In[43]:=
```
ScenarioA = {sa → 1,
    s11 → 45, s12 → 5, b1 → 50, x1 → 100, s1 → 10,
    s21 → 10, s22 → 90, b2 → 0, x2 → 100, s2 → 10,
    eta11 → .2, eta21 → .2, eta12 → .2, eta22 → .2};
ScenarioB = {sa → 1,
    s11 → 45, s12 → 5, b1 → 50, x1 → 100, s1 → 10,
    s21 → 10, s22 → 90, b2 → 0, x2 → 100, s2 → 10,
    eta11 → .1, eta21 → .3, eta12 → .2, eta22 → .2};
ScenarioC = {sa → 1,
    s11 → 45, s12 → 5, b1 → 50, x1 → 100, s1 → 10,
    s21 → 40, s22 → 60, b2 → 0, x2 → 100, s2 → 10,
    eta11 → 0, eta21 → .2, eta12 → 0, eta22 → 0};
ContourPlot[{
  Evaluate[LProfiled /. ScenarioA ] == 1.15,
  Evaluate[LProfiled /. ScenarioB ] == 1.15,
  Evaluate[LProfiled /. ScenarioC ] == 1.15,
  Evaluate[leffProfiled /. ScenarioA ] == 1.15,
  Evaluate[leffProfiled /. ScenarioB ] == 1.15,
  Evaluate[leffProfiled /. ScenarioC ] == 1.15
 },
 {mu1, .5, 1.8}, {mu2, 0.5, 1.8}, ContourLabels → True,
 PlotRange → {{0.5, 1.8}, {0.3, 2.2}}]
```

Out[46]=